

Parametrized Empirical Interpolation of Nonlinear Implicit Evolution Operators

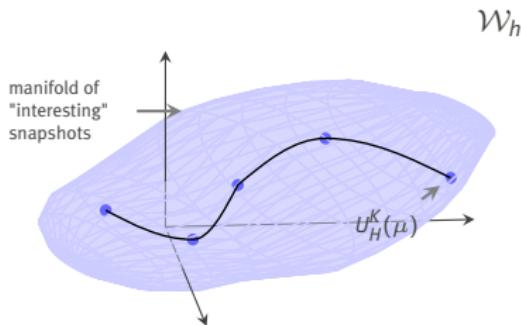
Reduced Basis Method

RB Scenario:

- ▶ Parametrized partial differential equations for (**non-stationary**) problems
- ▶ Applications relying on **time-critical** or many **repeated** simulations, e.g. design, control, optimization applications.

Goals:

- ▶ **Offline-/Online** decomposition
- ▶ Efficient reduced simulations
- ▶ A posteriori error control



References: [Patera&Rozza, 2006],
[Haasdonk et al., 2008]

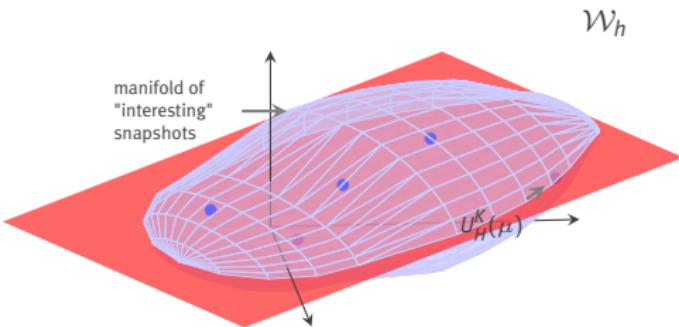
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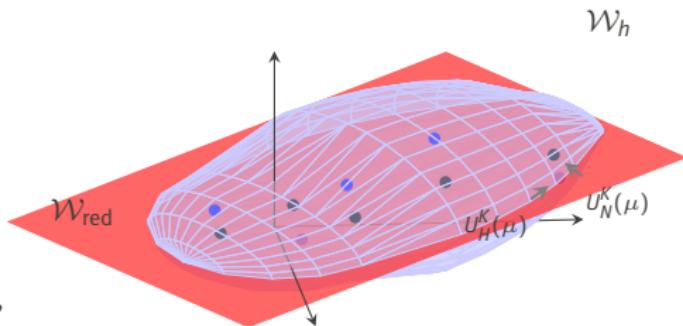
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Parametrized Evolution Equation

Analytical Formulation

For $\mu \in \mathcal{P} \subset \mathbb{R}^p$, find $u : [0, T_{\max}] \rightarrow \mathcal{W}_h \subset L^2(\Omega)$, s.t.

$$\partial_t u(t) - \mathcal{L}(\mu)[u(t)] = 0, \quad u(0) = u_0(\mu)$$

plus (parameter dependent) boundary conditions.

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plus (parameter dependent) boundary conditions.

Discretization (implicit/explicit with Newton scheme)

For $\mu \in \mathcal{P}$ find $\{u_h\}_{k=0}^K \subset \mathcal{W}_h \subset L^2(\Omega)$, s.t.

$$u_h^{k+1} := u_h^{k+1, \nu_{\max}(k)}, \quad u_h^0 := P_h[u_0(\mu)]$$

with Newton iteration

$$u_h^{k+1,0} := u_h^k, \quad u_h^{k+1,\nu+1} := u_h^{k+1,\nu} + \delta_h^{k+1,\nu+1},$$
$$\left(\text{Id} + \Delta t \mathbf{D} \mathcal{L}_h^I|_{u_h^{k+1,\nu}} \right) [\delta_h^{k+1,\nu+1}] = u_h^k - u_h^{k+1,\nu} - \Delta t \left(\mathcal{L}_h^I [u_h^{k+1,\nu}] + \mathcal{L}_h^E [u_h^k] \right).$$

Empirical interpolation: Idea

General operator approximation

Approximate operator evaluations

parameter de-
pendent

parameter inde-
pendent

$$\mathcal{L}_h(\mu) [u_h^k(\mu)] \approx \mathcal{I}_M [\mathcal{L}_h(\mu)] [u_h^k(\mu)] = \sum_{m=1}^M l_m(\mu) [u_h^k(\mu)] \xi_m,$$

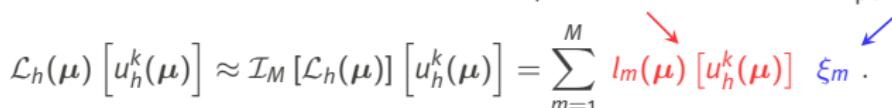
where $l_m(\mu) : \mathcal{W}_h \rightarrow \mathbb{R}$ are efficiently computable functionals and ξ_m collateral reduced basis functions.

Empirical interpolation: Idea

Approximate operator evaluations

$$\mathcal{L}_h(\boldsymbol{\mu}) \left[u_h^k(\boldsymbol{\mu}) \right] \approx \mathcal{I}_M [\mathcal{L}_h(\boldsymbol{\mu})] \left[u_h^k(\boldsymbol{\mu}) \right] = \sum_{m=1}^M l_m(\boldsymbol{\mu}) \left[u_h^k(\boldsymbol{\mu}) \right] \xi_m.$$

parameter dependent parameter independent



Empirical interpolation [Barrault et al, 2004]

- collateral reduced basis \mathcal{W}_M made out of operator evaluations $\mathcal{L}_h(\boldsymbol{\mu}_m) \left[u_h^{k_m}(\boldsymbol{\mu}_m) \right], m = 1, \dots, M$ for **suitably chosen** parameters $\boldsymbol{\mu}_m \in \mathcal{P}$ and time steps k_m . (Greedy search)
- coefficient functionals $l_m(\boldsymbol{\mu}) := \mathcal{L}_h(\boldsymbol{\mu}) [\cdot](x_m)$ are exact operator evaluations at **interpolation points** $\{x_m\}_{m=1}^M$.

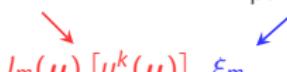
Empirical interpolation: Idea

Approximate operator evaluations

$$\mathcal{L}_h(\boldsymbol{\mu}) \left[u_h^k(\boldsymbol{\mu}) \right] \approx \mathcal{I}_M [\mathcal{L}_h(\boldsymbol{\mu})] \left[u_h^k(\boldsymbol{\mu}) \right] = \sum_{m=1}^M l_m(\boldsymbol{\mu}) \left[u_h^k(\boldsymbol{\mu}) \right] \xi_m.$$

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Empirical interpolation [Barrault et al, 2004]

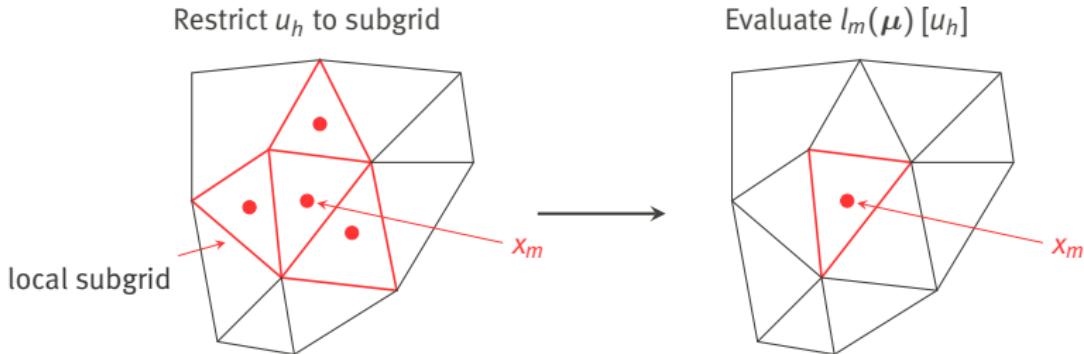
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- coefficient functionals $l_m(\boldsymbol{\mu}) := \mathcal{L}_h(\boldsymbol{\mu}) [\cdot](x_m)$ are exact operator evaluations at **interpolation points** $\{x_m\}_{m=1}^M$.
- CRB functions ξ_m are nodal in interpolation points, such that $\xi_m(x_n) = \delta_{nm}$.

Online evaluations

Efficient evaluations of $l_m(\mu)$

The coefficient functionals $l_m(\mu) = \mathcal{L}_h(\mu)[\cdot](x_m)$ can be computed efficiently during **online** phase, if

- ▶ operator has localized structure (**small stencil**) and
- ▶ local geometry information is precomputed in **offline** phase.



Collateral reduced basis generation

CRB extension algorithm

$m \leftarrow 0, q_0 \leftarrow 0$

repeat

▷ Initialization.

until $\|r_m\| \leq \varepsilon_{\text{tol}}$ or $m = M_{\max}$

Collateral reduced basis generation

CRB extension algorithm

```
m ← 0, q0 ← 0                                ▷ Initialization.  
repeat  
    for  $u_h \in L_{\text{train}}$  do  
         $u_h^* \leftarrow \arg \inf_{v_h \in \text{span}\{q_i\}_{i=1}^m} \|u_h - v_h\|$ .      ▷ Find the best approximation.  
         $u_m \leftarrow \arg \sup_{u_h \in L_{\text{train}}} \|u_h - u_h^*\|$ .      ▷ Find approximation with worst error.  
    end for  
  
until  $\|r_m\| \leq \varepsilon_{\text{tol}}$  or  $m = M_{\text{max}}$   
  
▶ Use  $L^\infty - \|\cdot\|$  or  $L^2 - \|\cdot\|$ 
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Collateral reduced basis generation

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    end for  
     $r_m \leftarrow u_m - \mathcal{I}_m[u_m]$           ▷ Compute the residual between  $u_m$  and its interpolant.  
     $x_m \leftarrow \arg \sup_{x \in X_H} |r_m(x)|$       ▷ Find new interpolation point.  
     $q_m \leftarrow \frac{r_m}{r_m(x_m)}$                   ▷ Find new CRB function.  
     $m \leftarrow m + 1$   
until  $\|r_m\| \leq \varepsilon_{\text{tol}}$  or  $m = M_{\text{max}}$ 
```

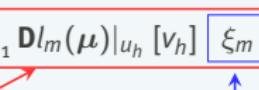
- ▶ Use $L^\infty - \|\cdot\|$ or $L^2 - \|\cdot\|$
- ▶ For notation: nodal basis $\xi := \{\xi_m\}_{m=1}^M$ made out of $\{q_m\}_{m=1}^M$

Derivative of empirical interpolation

Observation

$$\mathbf{D}\mathcal{I}_M [\mathcal{L}_h(\mu)]|_{u_h}[v_h] = \sum_{m=1}^M \mathbf{D}l_m(\mu)|_{u_h}[v_h] \boxed{\xi_m}$$

parameter dependent parameter independent



Derivative of empirical interpolation

$$\mathbf{D}\mathcal{I}_M [\mathcal{L}_h(\mu)]|_{u_h}[v_h] = \boxed{\sum_{m=1}^M \mathbf{D}l_m(\mu)|_{u_h}[v_h]} \boxed{\xi_m}$$

↑
parameter dependent ↑
parameter independent

Coefficient functionals

\mathcal{W}_h is finite dimensional

$$\mathbf{D}l_m(\mu)|_{u_h}[v_h] = \sum_{m=1}^M \sum_{i=1}^H \frac{\partial}{\partial \psi_i} l_m(\mu)[u_h](\underline{v}_{h,i})$$

Derivative of empirical interpolation

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Coefficient functionals

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\mathcal{L}_h has local stencil

Derivative of empirical interpolation

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\uparrow

\mathcal{L}_h has local stencil

Note: $\text{card}(I_{x_m}) < C$ for all $m = 1, \dots, M$. \Rightarrow Complexity still $\mathcal{O}(M)$.

Reduced basis method for nonlinear schemes

- ▶ Generate reduced basis space $\mathcal{W}_{\text{red}} := \text{span} \{ \varphi_i \}_{i=1}^N \subset \mathcal{W}_h$ with **POD-Greedy** algorithm.
- ▶ $P_{\text{red}} : \mathcal{W}_h \rightarrow \mathcal{W}_{\text{red}}$ Galerkin projection onto $\mathcal{W}_{\text{red}} \subset \mathcal{W}_h$
- ▶ Offline-/online decomposition of operators:

$$(P_{\text{red}}[u_{h,0}(\mu)])_n = \sum_{q=1}^{Q_{u0}} \sigma_{u0}^q(\mu) \left[\int_{\Omega} u_0^q \varphi_n \right] \quad \begin{matrix} \text{assuming: } u_0(\mu) = \sum_{q=1}^{Q_{u0}} \sigma_{u0}^q(\mu) u_0^q \\ \text{online} \qquad \qquad \text{offline} \end{matrix}$$

$$\left(\mathcal{L}'_{\text{red}}(\mu) \left[u_{\text{red}}^k(\mu) \right] \right)_n = \sum_{m=1}^M l_m'(\mu) [u_{\text{red}}] \left[\int_{\Omega} \xi_m \varphi_n \right] \quad \begin{matrix} \text{online} \qquad \qquad \text{offline} \end{matrix}$$

$$\left(\mathbf{D}\mathcal{L}'_{\text{red}}(\mu)|_{u_{\text{red}}} [\delta_{\text{red}}] \right)_n = \sum_{m=1}^M \frac{\partial}{\partial \psi_i} l_m'(\mu) [u_{\text{red}}] \left[\int_{\Omega} \xi_m \varphi_n \right] \quad \begin{matrix} \text{online} \qquad \qquad \text{offline} \end{matrix}$$

Reduced basis method for nonlinear schemes

Projection of Operators:

- $P_{\text{red}} : \mathcal{W}_h \rightarrow \mathcal{W}_{\text{red}}$ Galerkin projection onto $\mathcal{W}_{\text{red}} \subset \mathcal{W}_h$
- $\mathcal{L}_{\text{red}}^I := P_{\text{red}} \circ \mathcal{I}_M \circ \mathcal{L}_h^I$
- $\mathcal{L}_{\text{red}}^E := P_{\text{red}} \circ \mathcal{I}_M \circ \mathcal{L}_h^E$

Reduced simulation

For $\mu \in \mathcal{P}$ find $\{u_{\text{red}}\}_{k=0}^K \subset \mathcal{W}_{\text{red}}$, s.t.

$$u_{\text{red}}^{k+1} := u_{\text{red}}^{k+1, \nu_{\max}(k)}, \quad u_{\text{red}}^0 := P_{\text{red}} [u_{h,0}(\mu)]$$

with Newton iteration

$$\begin{aligned} u_{\text{red}}^{k+1,0} &:= u_{\text{red}}^k, & u_{\text{red}}^{k+1,\nu+1} &:= u_{\text{red}}^{k+1,\nu} + \delta_{\text{red}}^{k+1,\nu+1}, \\ \left(\text{Id} + \Delta t \mathbf{D} \mathcal{L}_{\text{red}}^I \big|_{u_{\text{red}}^{k+1,\nu}} \right) \left[\delta_{\text{red}}^{k+1,\nu+1} \right] &= u_{\text{red}}^k - u_{\text{red}}^{k+1,\nu} - \Delta t \left(\mathcal{L}_{\text{red}}^I \left[u_{\text{red}}^{k+1,\nu} \right] + \mathcal{L}_{\text{red}}^E \left[u_{\text{red}}^k \right] \right). \end{aligned}$$

A posteriori error estimator

Theorem (A posteriori error estimator)

Assumptions:

- ▶ Operators and $\mathbf{D}\mathcal{L}_h^I$ are Lipschitz-continuous.
- ▶ $\mathbf{D}\mathcal{L}_h^I$ has bounded inverse
- ▶ Empirical interpolations exact for larger CRB space $\mathcal{W}_{M+M'}$ and $P_h[u_0(\mu)] \in \mathcal{W}_{\text{red}}$

Then:

$$\|u_{\text{red}}^k(\mu) - u_h^k(\mu)\| \leq \Delta_{N,M}^k(\mu) \quad \text{with } \Delta_{N,M}(\mu) := \sum_{i=0}^{k-1} \sum_{j=1}^{\nu_{\max}(i)} \bar{\Delta}^{i,j}$$

recursively defined through the Newton step error estimator

$$\begin{aligned} \bar{\Delta}^{k+1,j+1} := \Delta t & \left(C_1 \bar{\Delta}^{k_1,\nu} + C_2 \bar{\Delta}^{k+1,\nu} + \|\delta_{\text{red}}^{k+1,\nu+1}\| + \right. \\ & \left. \|R_{D,M}^{k+1,\nu+1}\| + \|R_{I,M}^{k+1,\nu}\| + \|R_{E,M}^{k+1,0}\| + \|R^{k+1,\nu}\| \right). \end{aligned}$$

A posteriori error estimator

Theorem (A posteriori error estimator cont.)

Then:

$$\|u_{\text{red}}^k(\mu) - u_h^k(\mu)\| \leq \Delta_{N,M}^k(\mu) \quad \text{with } \Delta_{N,M}(\mu) := \sum_{i=0}^{k-1} \sum_{j=1}^{\nu_{\max}(i)} \bar{\Delta}^{i,j}$$

recursively defined through the Newton step error estimator

$$\begin{aligned} \bar{\Delta}^{k+1,j+1} := & \Delta t \left(C_1 \bar{\Delta}^{k_1,\nu} + C_2 \bar{\Delta}^{k+1,\nu} + \left\| \delta_{\text{red}}^{k+1,\nu+1} \right\| + \right. \\ & \left. \left\| R_{D,M}^{k+1,\nu+1} \right\| + \left\| R_{I,M}^{k+1,\nu} \right\| + \left\| R_{E,M}^{k+1,0} \right\| + \left\| R^{k+1,\nu} \right\| \right). \end{aligned}$$

The residuals $R_{*,M}$ measure the empirical interpolation error, e.g.

$$R_{I,M}^{k+1,\nu} := \sum_{m=M}^{M+M'} l_m' \left[u_{\text{red}}^{k+1,\nu} \right] \xi_m$$

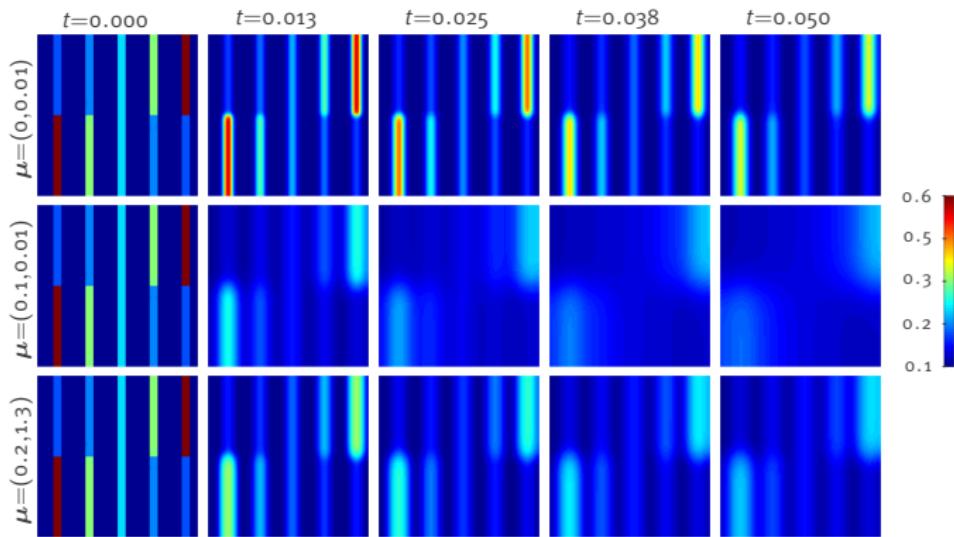
Numerical results: Nonlinear Diffusion

Problem definition:

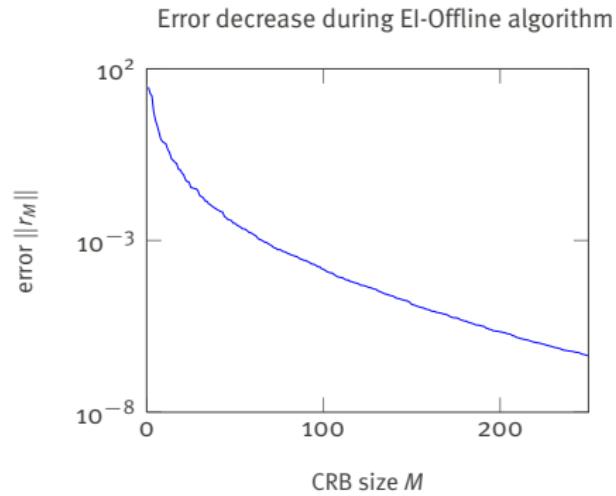
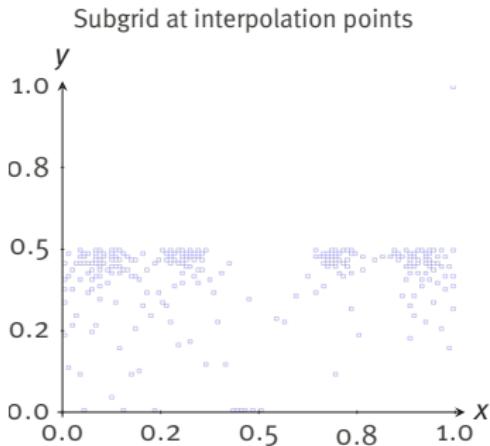
$$\partial_t u(t) - \nabla \cdot ((k_0 + mu(t)^p) \nabla u(t))$$

with homogeneous boundary conditions, $\mu = (m, p) \in [0, 0.3] \times [0.01, 2]$.

Sample trajectories:



Numerical results: Empirical interpolation of \mathcal{L}_h^I



Numerical Results

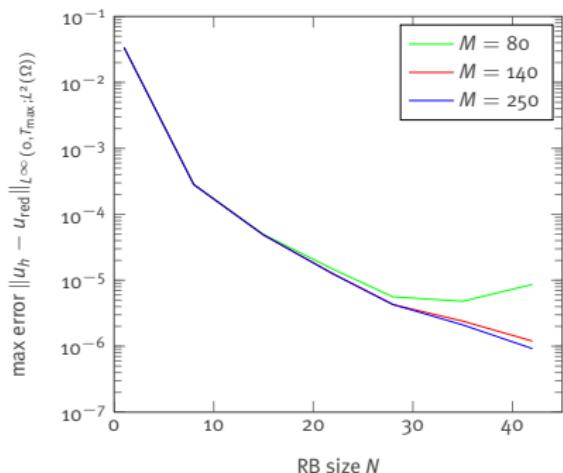


Figure: RB error convergence on 100 test samples

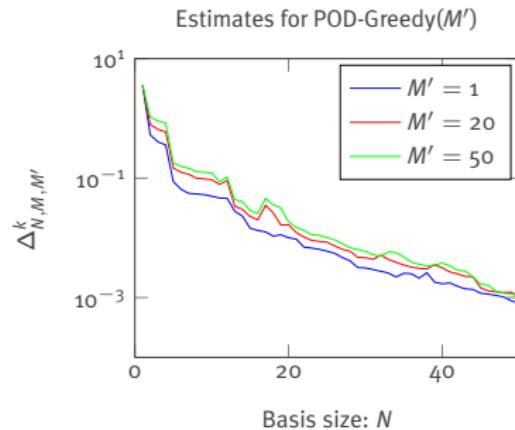
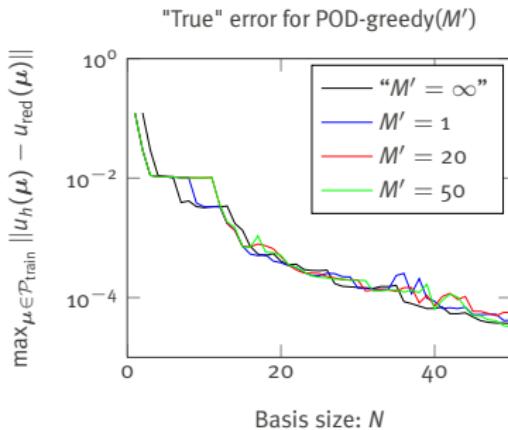
dimension	time[s]	error
H=10000	17.05	0
N=15M=84	1.67	$4.97 \cdot 10^{-5}$
N=42M=84	1.72	$8.65 \cdot 10^{-6}$
N=15M=139	1.93	$4.86 \cdot 10^{-5}$
N=28M=139	1.96	$4.29 \cdot 10^{-6}$
N=42M=139	2.01	$1.2 \cdot 10^{-6}$
N=15M=250	2.44	$4.87 \cdot 10^{-5}$
N=28M=250	2.48	$4.29 \cdot 10^{-6}$
N=42M=250	2.53	$9.21 \cdot 10^{-7}$

Table: average time measurements on 100 test samples

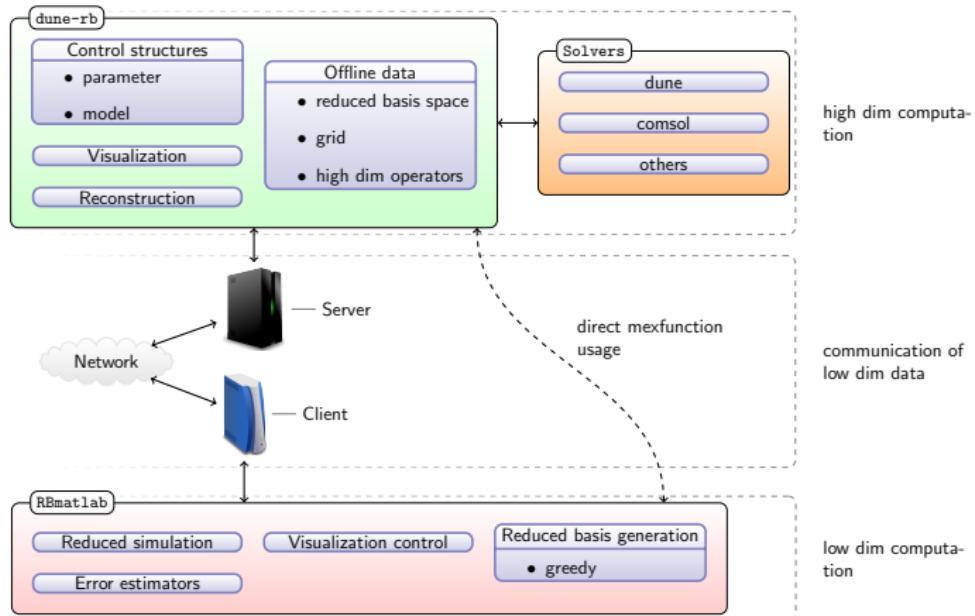
Number of base functions in \mathcal{W}_h : 10000
 Number of Newton steps ν_{\max} : $\approx 1 - 12$
 Time gain factor for online phase: $\approx 8 - 10$

Numerical results: A posteriori error estimator

POD-Greedy with efficient error control (explicit Burgers problem)



Software concepts (dune-rb/RBmatlab interface)



For further information see: <http://morepas.org>

Software concepts (dune-rb/RBmatlab interface)

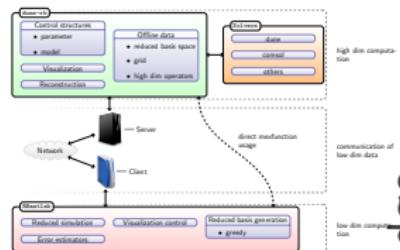
Goals:

- ▶ Access to open source implementations of “real world” problems.
- ▶ Testing the reduced basis methods on these implementations.

Status:

- ▶ Communication interface between rbmatlab and dune exists
- ▶ Example implementation: linear heat equation in Dune affinely parameter dependent structure. (No empirical interpolation necessary)
- ▶ Empirical interpolation of simple operators almost ready.

For further information see: <http://morepas.org>



References

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Version 1.0, Copyright MIT 2006, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering
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C. R. Math. Acad. Sci. Paris Series I, 2004, 339, 667-672
-  [Drohmann et al., 2009] M. Drohmann, B. Haasdonk and M. Ohlberger,
Reduced Basis Method for Finite Volume Approximation of Evolution Equations on Parametrized Geometries
Proceedings of ALGORITMY 2009, 111–120

Older results

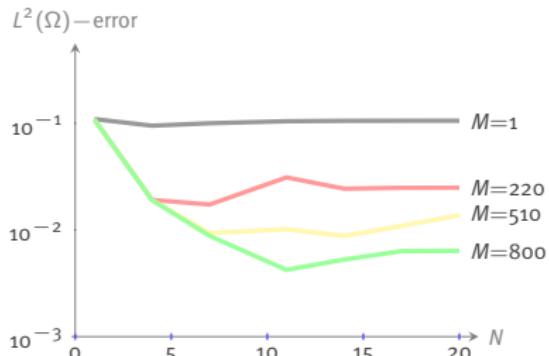


Figure: RB error convergence on 100 test samples

dimension	time[s]
$H=40000$	24.37
$N=7, M=267$	1.22
$N=7, M=800$	2.05
$N=14, M=267$	1.25
$N=14, M=800$	2.1
$N=20, M=267$	1.27
$N=20, M=800$	2.11

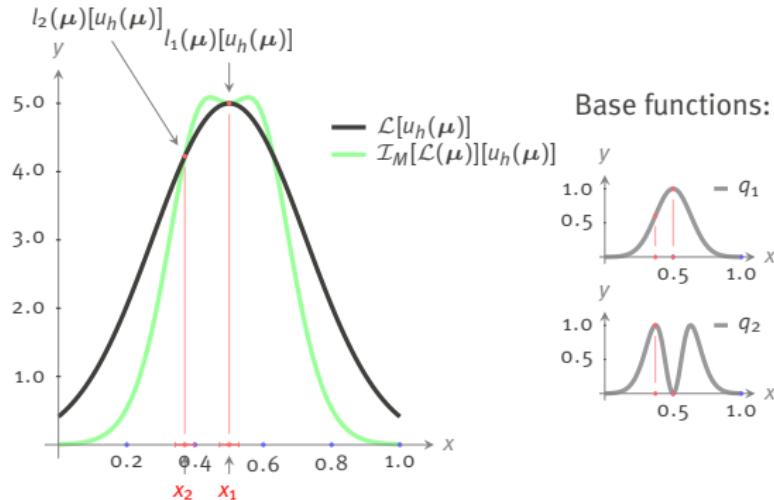
Table: average time measurements on 100 test samples

Number of base functions in \mathcal{W}_h : 40000
 Time gain factor for online phase: ≈ 10

Efficient evaluations of $l_m(\mu)$

The coefficient functionals $l_m(\mu) = \mathcal{L}_h(\mu)[\cdot](x_m)$ can be computed efficiently during **online** phase, if

- ▶ operator has localized structure (**small stencil**) and
- ▶ local geometry information is precomputed in **offline** phase.



Reduced basis generation

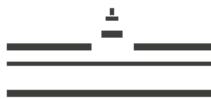
POD-greedy algorithm

- ▶ **Initialization:** Define an initial reduced basis \mathcal{W}_{N_0} and a finite training parameter set $M_{\text{train}} \subset \mathcal{P}$.

Reduced basis generation

POD-greedy algorithm

- ▶ **Initialization:** Define an initial reduced basis \mathcal{W}_{N_0} and a finite training parameter set $M_{\text{train}} \subset \mathcal{P}$.
- ▶ **Iterative extension of basis:**
 - ▶ Find $\boldsymbol{\mu}_{\max} := \arg \max_{\boldsymbol{\mu} \in M_{\text{train}}} \max_{k=0}^K \|u_{\text{red}}^k(\boldsymbol{\mu}) - u_h^k(\boldsymbol{\mu})\|$ (with efficient a posteriori error estimates).
 - ▶ Add principal components of projection error of trajectory $\left\{ u_{\text{red}}^k - u_h^k \right\}_{k=1}^K$ to reduced basis.
- ▶ **Stop:** if error is small enough.



Geometry transformation on heat equation

We look again at the non-stationary heat equation

$$\partial_t u(x, t; \mu) - a(\mu) \Delta u(x, t; \mu) = 0 \quad \text{in } \Omega(\mu) \times [0, T_{\max}].$$

Geometry transformation on heat equation

The reduced basis space must not depend on the parameter.

Therefore, we introduce a reference geometry $\hat{\Omega}$ and a **diffeomorphic** mapping $\Phi(\mu) : \hat{\Omega} \rightarrow \Omega(\mu)$ for every parameter.

We look again at the non-stationary heat equation

$$\partial_t u(x, t; \mu) - a(\mu) \Delta u(x, t; \mu) = 0 \quad \text{in } \Omega(\textcolor{red}{X}) \times [0, T_{\max}].$$

Geometry transformation

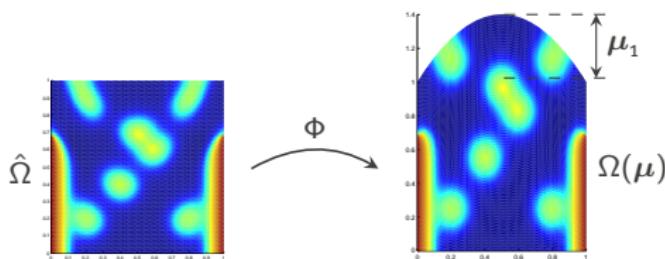
Transformed heat equation

The result is a PDE with (anisotropic) diffusion, convection and a reaction term:

$$\partial_t \hat{u} - a(\mu) \nabla \cdot (GG^t \nabla \hat{u}) + a(\mu) \nabla \cdot (v\hat{u}) - a(\mu)(\nabla \cdot v)\hat{u} = 0 \quad \text{in } \hat{\Omega} \times [0, T_{\max}],$$

with notations

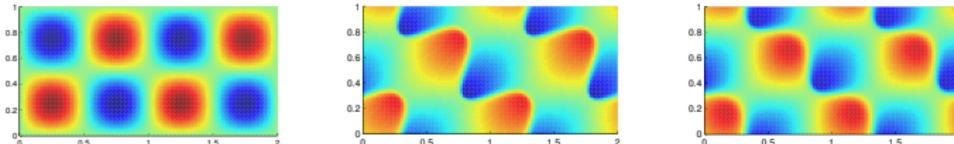
$$\begin{aligned}\hat{x} &:= \Phi^{-1}(x), & \hat{u}(\hat{x}, t) &:= u(\Phi(\hat{x}), t), \\ G(\hat{x}) &:= D\Phi^{-1}|_{\Phi(\hat{x})}, & v(\hat{x}) &:= G(\hat{x})(\nabla_{\hat{x}} \cdot G(\hat{x})).\end{aligned}$$



Numerical results: Empirical interpolation

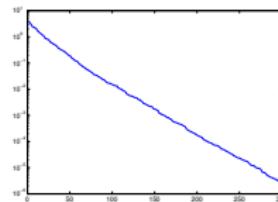
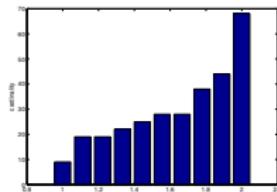
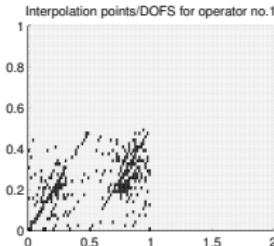
Burgers problem:

$\partial_t u - \nabla \cdot (\mathbf{v} u(\mu)^p) = 0$ with periodic boundary conditions, $\mu = p \in [1, 2]$



(i) initial data snapshot ($T = 0$), (ii) snapshot for $p = 2$ at $T = 0.3$, (iii) snapshot for $p = 1.5$ at $T = 0.3$

Empirical interpolation of L_E :



(i) interpolation points, (ii) frequency of parameter selection, (iii) EI error decrease